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LLNL-PROC-551411

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H. Hsieh, J. Sanz-Argent, G. Petitpas, M. Havstad, D. Flowers

April 23, 2012

ASME V&V Symposium
Las Vegas, NV, United States
May 2, 2012 through May 4, 2012

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Sensitivity analysis of large system of chemical kinetic parameters for engine combustion simulation

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H. Hsieh, J. Sanz-Argent*, G. Petitpas, M. Havstad, D. Flowers

* Grupo de Combustibles y Motores - Universidad de Castilla-La Mancha, Spain

Lawrence Livermore National Laboratory

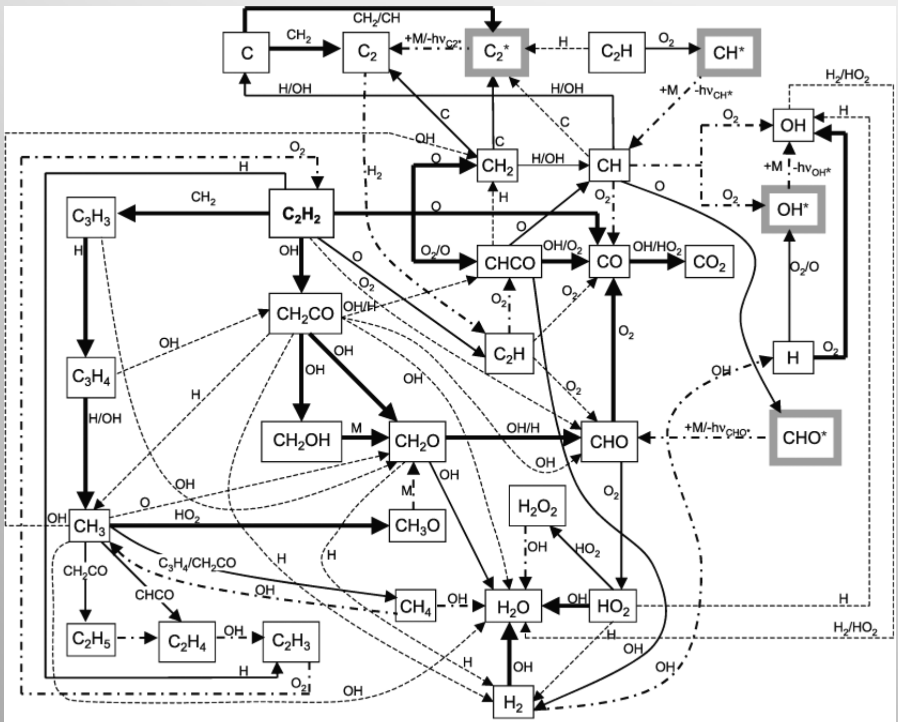
LLNL-PRES-XXXXXX

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Outline

- What problem are we solving?
- Why are we doing this study?
- Approach
- Conclusion

Kinetic mechanisms include 10^3 to 10^5 parameters, carrying some uncertainty



C_2H_2 oxidation, From Marques et al, J. Braz. Chem. Soc. vol.17 no.2 São Paulo Mar./Apr. 2006

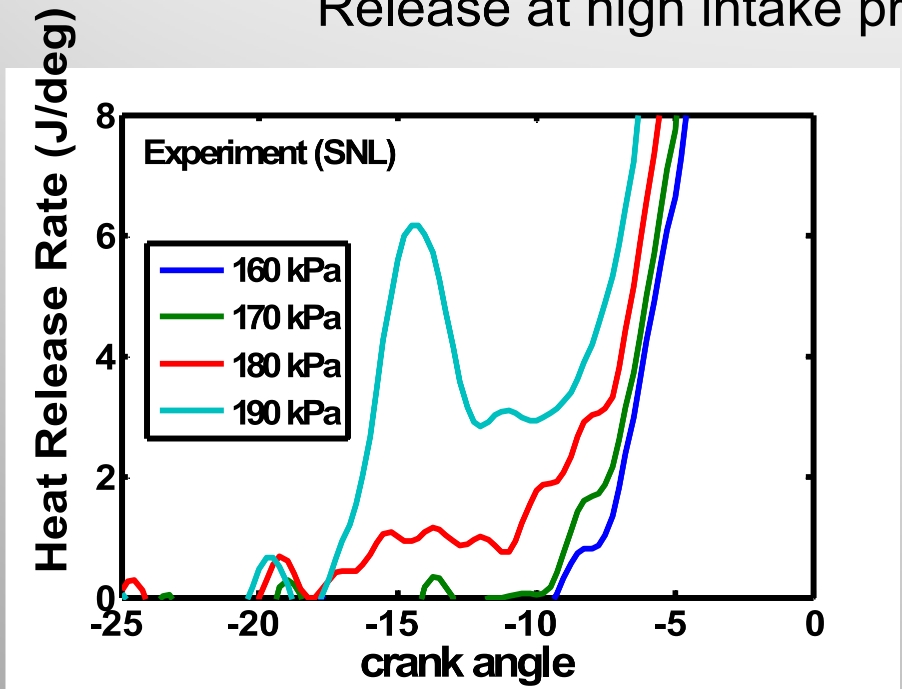
- A kinetic mechanism describes all the oxidation paths from a **fuel** to **oxidation**, using elementary chemical reactions whose rate is controlled by up to 5 kinetic parameters each

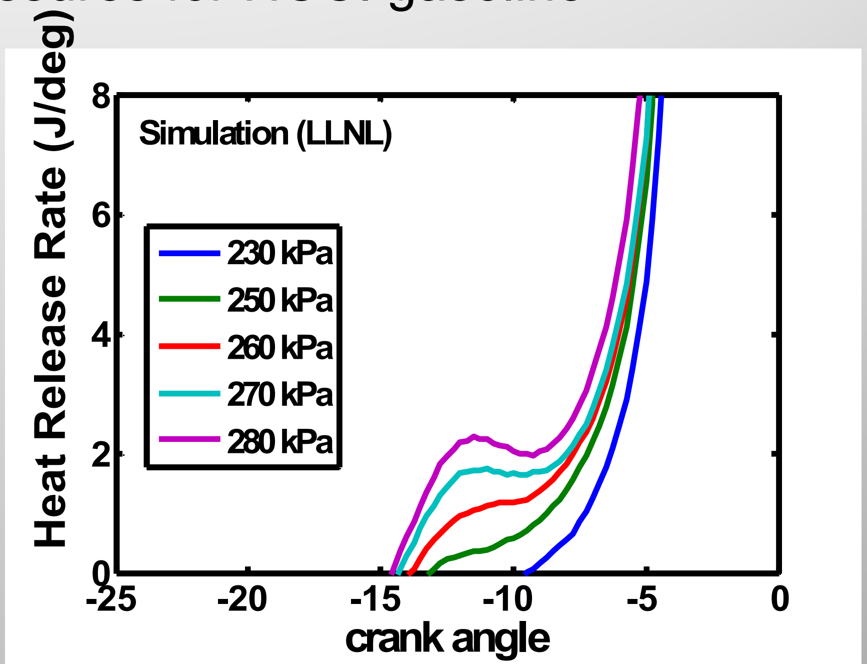
- Kinetic parameters known through:
  - Validation using macroscopic parameters (ignition delay, flame speed, etc.)
  - Similarity rules
  - Optimization of the Arrhenius parameters

$$k = A.T^{\beta}\exp\left(\frac{-Ea}{RT}\right)$$

Existing kinetics schemes fail to predict some new combustion concepts

Simulations underestimate Low Temperature Heat Release at high intake pressures for HCCI gasoline





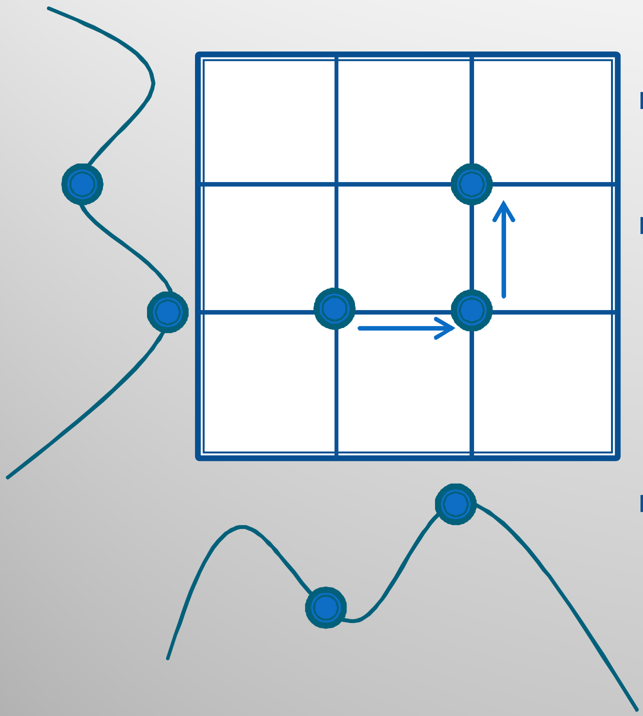
<u>Experiments</u> show low temperature heat release as low as **180 kpa**

<u>Simulations</u> show low temperature heat release only above **230 kpa**

Sensitivity analysis could improve the accuracy of large kinetics mechanisms

- <u>Objectives</u> : Selection of system parameters from humongous (4000+) to a handful, using the state-of-the-art sensitivity method.
  - Please note that the large kinetics mechanism represents a ‘reduced’ model based on subject expert judgment over the original model with 23000+ parameters.
- Step 1: Screening study using Morris-One-At-a-Time (MOAT)
- Step 2: A more detailed sensitivity analysis using variance-based method, Variance of Conditional Expectation (VCE).

Morris' Method



- It is a "one-factor-at-a-time" method.
- Each input factor may assume a discrete number of values, called levels (p=4 as shown)
- Two measures are proposed for each factor: mean (to estimate the overall first order effect, or main effect) and standard deviation (to assess second or higher order effect)

$$y = f(x_1, x_2, \cdots, x_N)$$

$$= f_0 + \frac{\partial f}{\partial x_i}(x_{10}, x_{20}, \cdots, x_{N0}) + \frac{\partial^2 f}{\partial x_i \partial x_j}(x_{10}, x_{20}, \cdots, x_{N0}) + H.O.T.$$

MOAT Algorithm

- Let N be the number of parameters, we defined a design space Ω as
  - $\Omega=\{X_i \in D_i \subset R, i=1,2,3,\ldots,N\}$
- Step 1: choose an initial point in Ω
  - Generating a random sequence with replacement from {1,…,p} where p is the number of grid of each parameters
- Step 2: generate a random path in Ω
  - Generating a random sequence w/o replacement from {1,…,N}
- Step 3: On each entry of step 2, randomly chose binary integer number between (+1 or -1). This represents the directions of perturbation of each parameters.
- Repeating step 1 to step 3 for n times where n is the desired number of sampling points

Variance of Conditional Expectation

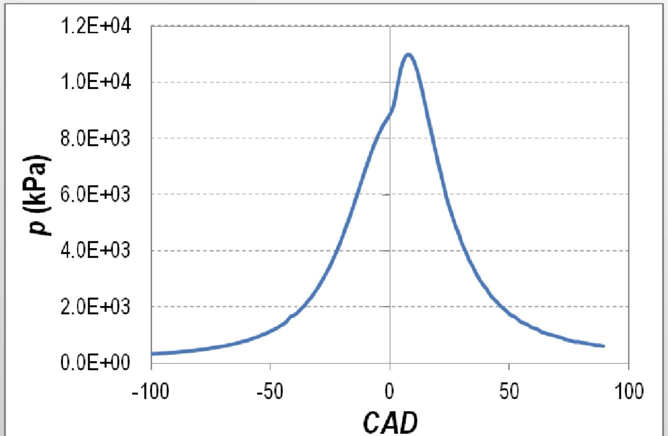
- For a more detailed sensitivity analysis in this study, we applied VCE
  - A variance-based method
  - Let Y be the output and X be the input parameters,
    - $V[Y] = E[V[Y|X]] + V[E[Y|X]]$

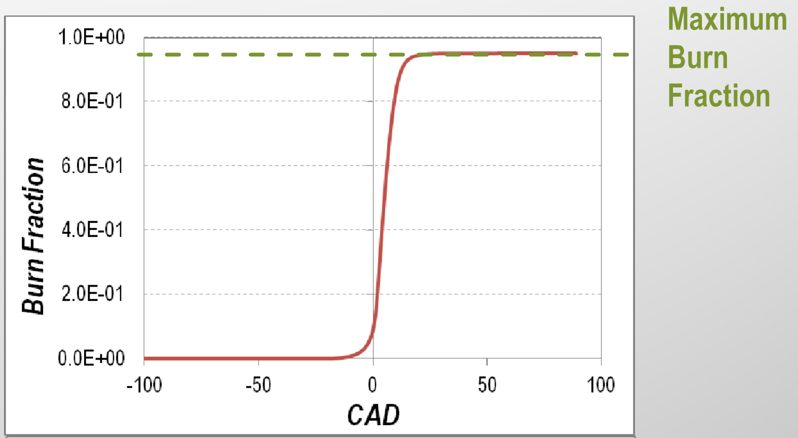
    Total variance of output response can be decomposed in terms of expected value of conditional variance ($E[V[Y|X]]$) and variance of conditional expectation ($V[E[Y|X]]$) .

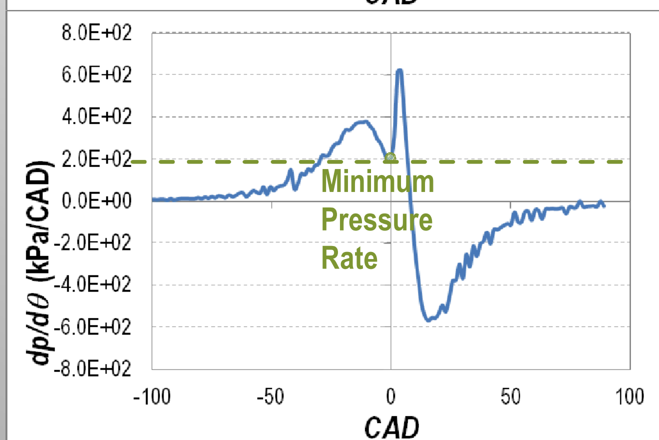
    The ratio of $V[E[Y|X]]$ to $V[Y]$ is quantify the importance of X to the output response.

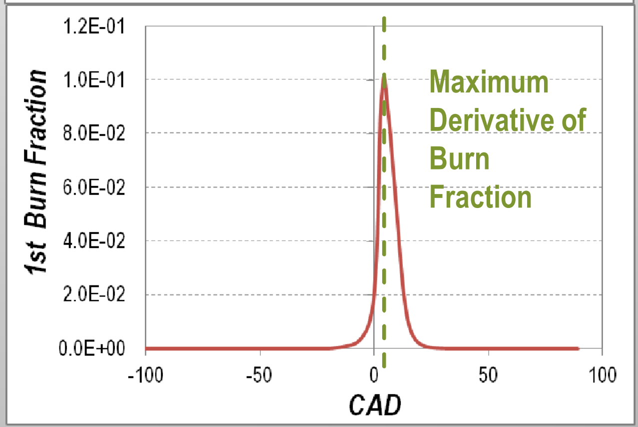
    For VCE, we used Latin Hypercube sampling. (for 84 parameters, we used 37800 samples.)

Outputs are carefully chosen in order to meet sensitivity analysis scope



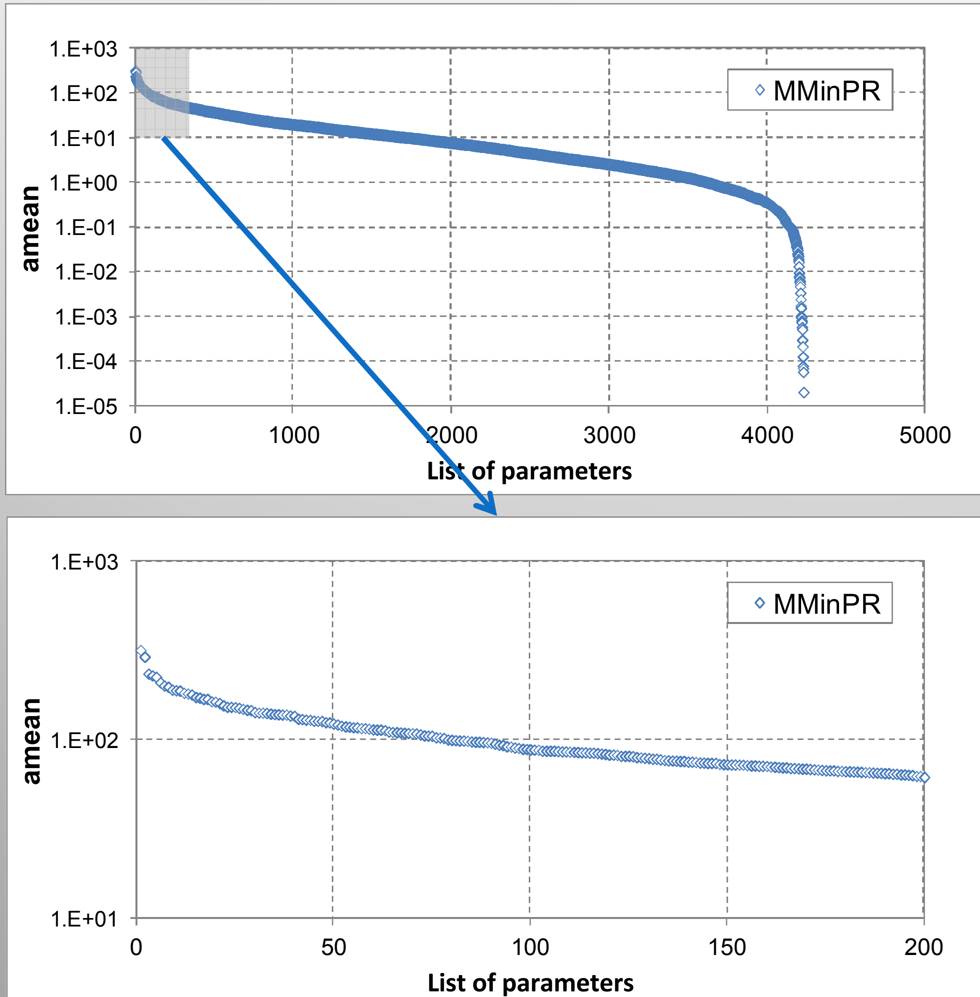






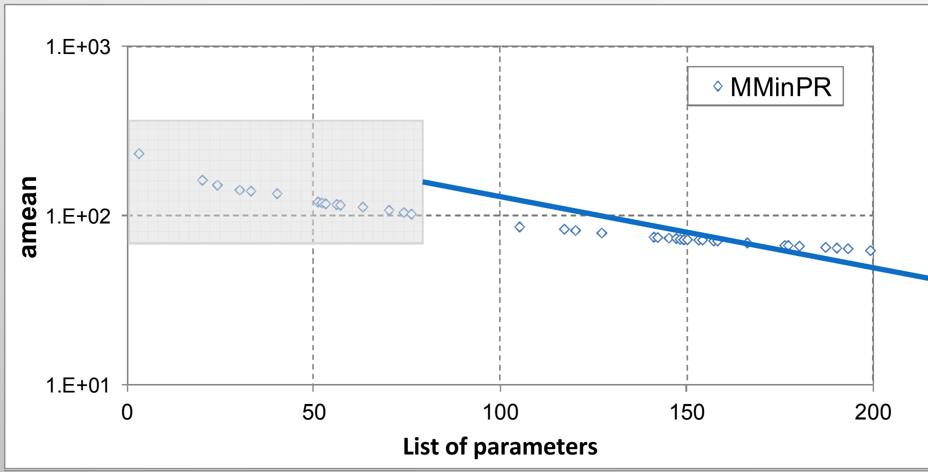
Magnitude of the Minimum pressure rate (MMinPR): Low temperature heat release
Magnitude of the Maximum Burn Fraction (MMaxBF): Total amount of heat released
Angle of the maximum derivative of the burn fraction (AMaxDBF): Main ignition timing

Step 1: screening, MOAT method using 25 sampling path



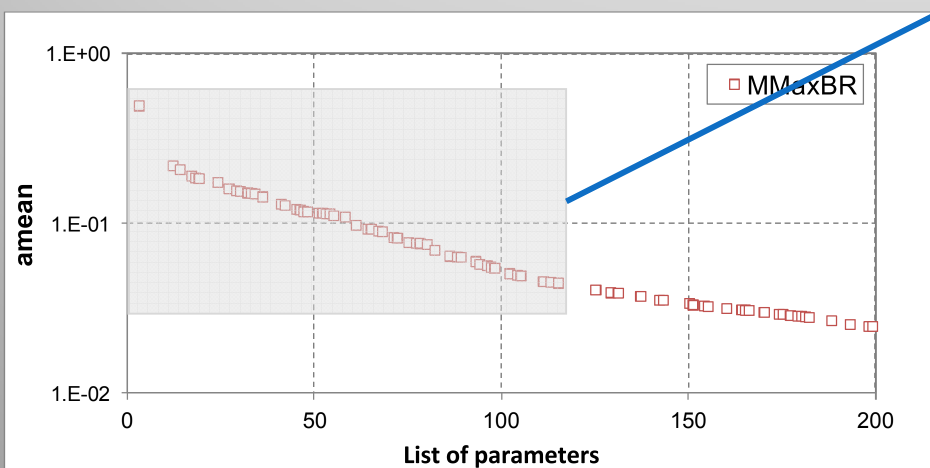
- After 500,000 CPU hours later and many man hours, we collected 25 samples (each sample requires 4258 simulation).
- This plot show the MOAT results of Magnitude of the Minimum Pressure Rate.
- The gradient of parameters decreases gradually. This makes screening process very difficult. Ideally, we would like to distinguish "A" parameters from the population.

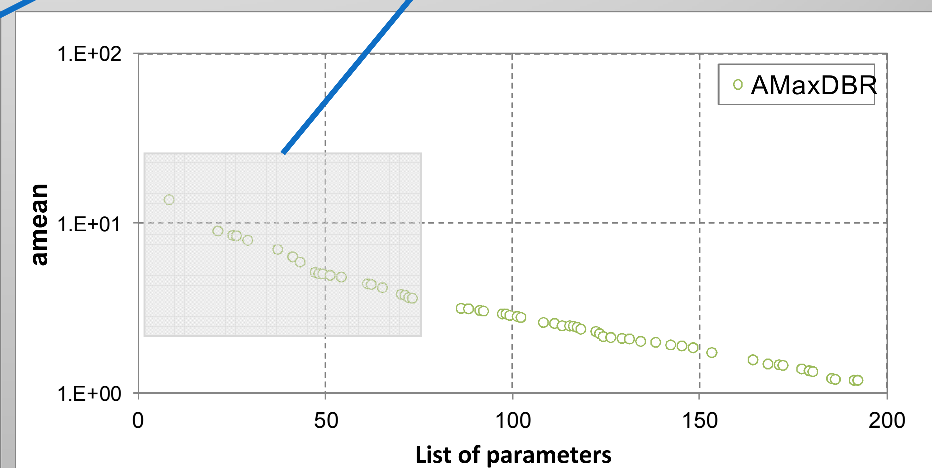
Step 1: screening, MOAT method using 25 sampling path



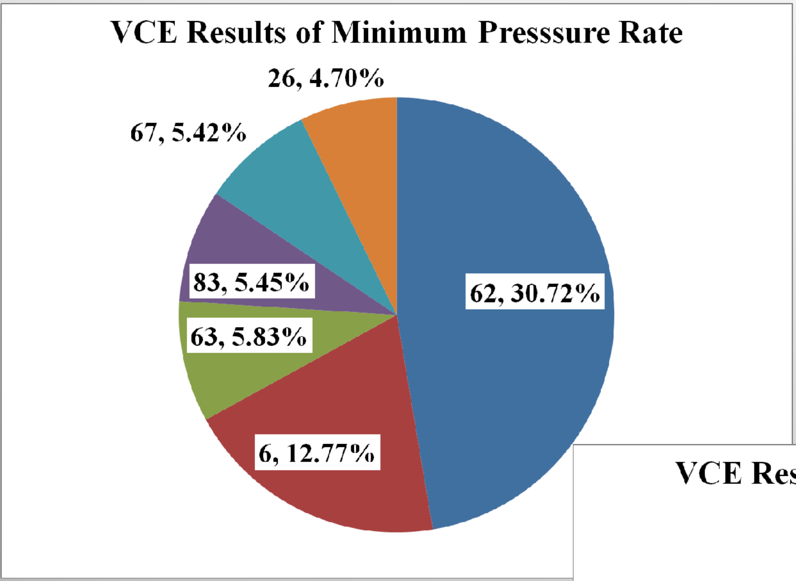
- No parameter from C0-C4 submechanism
  - -Included in most kinetic mechanisms
- Large mean/amean rate
  - - Changes in the main oxidation paths

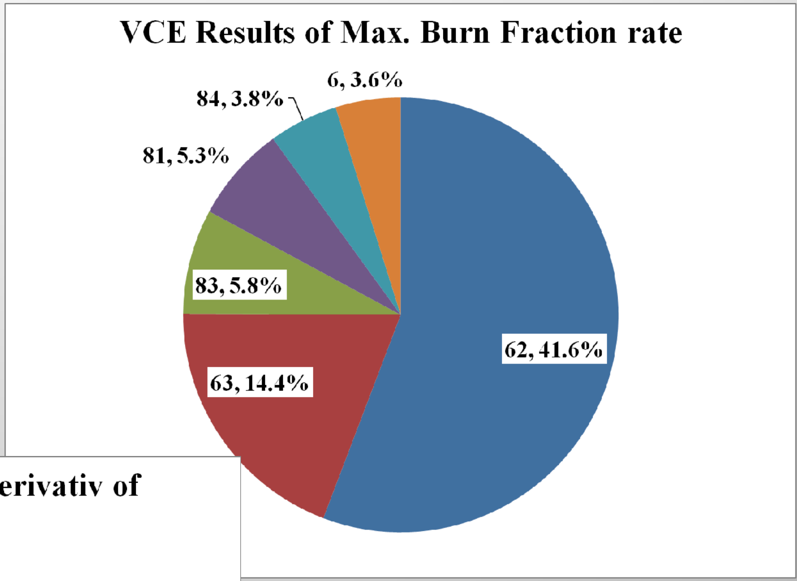
84 parameters

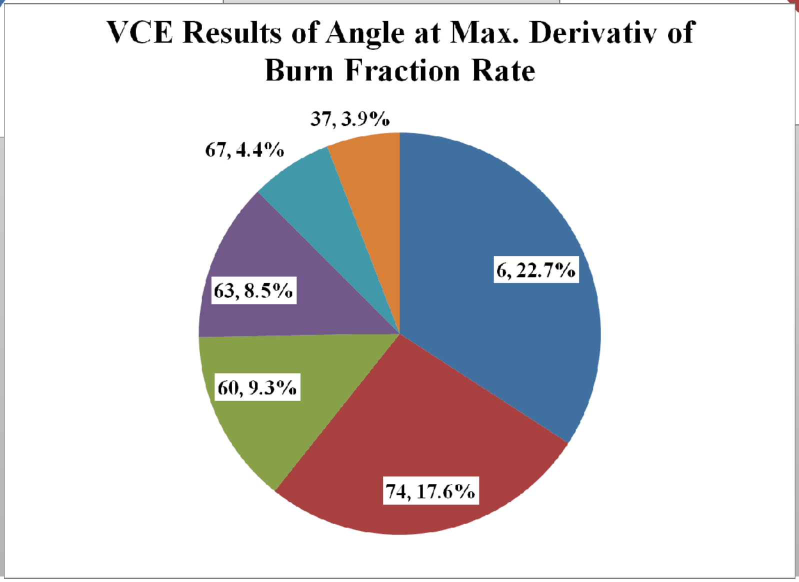




Step 2: VCE Results







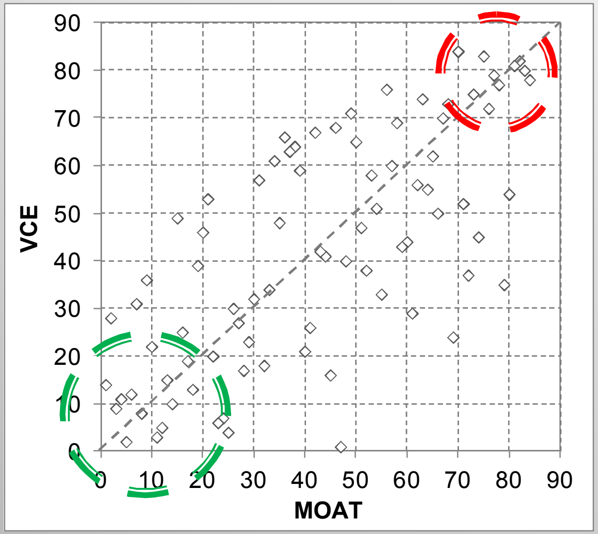
Parameter selection results based on VCE

- 2 output response: Magnitude of minimum pressure rate and angle at max. derivative of burn fraction rate.
- Both outputs are related: ↑ MMinPR ↓ AMaxDB
- Chemistry of all the surrogate compounds represented
- Selection of 8 parameters

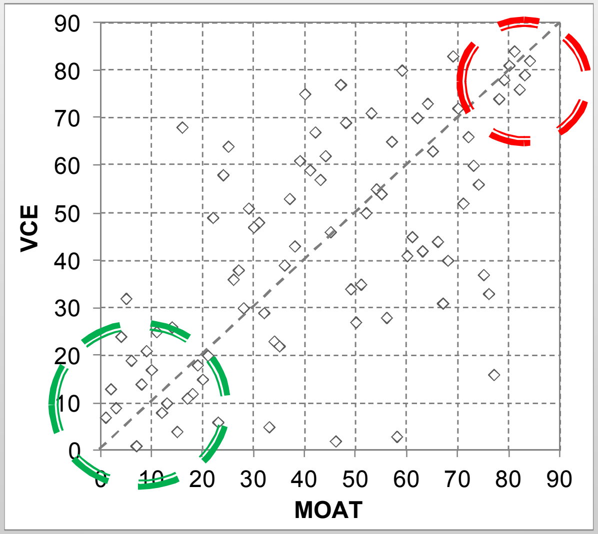
#	Parameter	Reaction
81	reg371603	C5H10-1+O2<=>C5H91-3+HO2
83	reg502503	C7H14OOH1-3O2<=>C7H14OOH1-3+O2
54	reg567603	HOC6H4CH3+O2<=>OC6H4CH3+HO2
38	reg554302	C6H5CH3+OH<=>C6H5CH2J+H2O
63	reg548903	C6H5OH+O2<=>C6H5OJ+HO2
67	reg244402	XC7H14+HO2<=>XC7H13-Z+H2O2
6	reg331202	CC8H17O2<=>CC8H17+O2
74	reg323403	IC8H18+HO2<=>AC8H17+H2O2

Comparison of SA results from MOAT and VCE

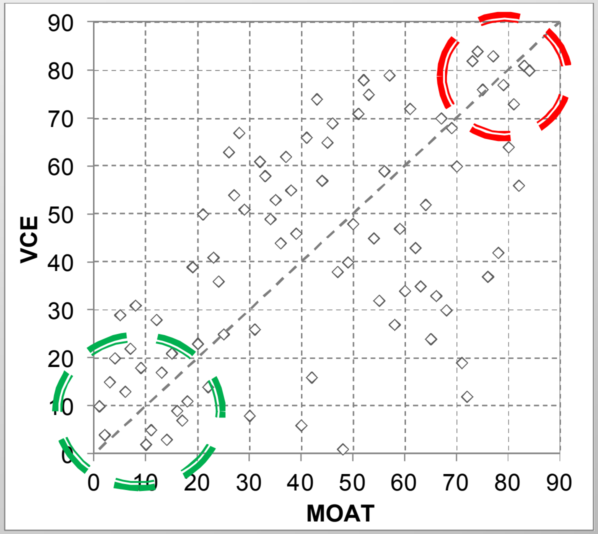
MMinPR



MMaxBR



AMaxDBR



- Number of parameters below + 1 (e.g. value of the most sensitive one is 84)
- Reasonable consistency at the extremes, especially for the most sensible parameters
- Poor consistency in some cases

Conclusion/Future

- In this study, we applied the state-of-the-art sensitivity methods to downselect system parameters from 4000+ to 8.
  - (23000+ -> 4000+ -> 84 -> 8)
- This analysis procedure paves the way for future works:
  - calibrate the system response using existed experimental observations, and
  - predict future experiment results, using the calibrated system